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Temperature-dependent density profiles of trapped boson-fermion mixtures

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Abstract

We present a semiclassical three-fluid model for a Bose-condensed mixture of interacting Bose and Fermi gases confined in harmonic traps at finite temperature. The model is used to characterize the experimentally relevant behaviour of the equilibrium density profile of the fermions with varying composition and temperature across the onset of degeneracy, for coupling strengths relevant to a mixture of ^{39}K and ^{40}K atoms.

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The achievement of Bose-Einstein condensation (BEC) in trapped gases of ^{87}Rb [1], ^{23}Na [2] and ^{7}Li [3] has provided new impulse to the study of many-body and quantum statistical effects in dilute fluids at very low temperature. The formation of coexisting condensates by sympathetic cooling in a mixture of Rb atoms in two different internal states has also been achieved [4]. Trapping of fermionic species has been reported for ^{6}Li [5] and ^{40}K [6]. Trapped mixtures of bosonic and fermionic species are expected to become accessible to experiment in the near future.

The density profiles of the separate fermionic and bosonic species in such mixtures can in principle be experimentally resolved. With this perspective we present in this work a semiclassical three-fluid model extending our earlier studies of the condensate fraction and internal energy of a trapped interacting Bose gas [7, 8] to a Bose-condensed mixture of interacting Bose and Fermi gases confined in a spherically symmetric trap at finite temperature. We assume that the mixture is in full thermal equilibrium: the efficiency of a Bose condensate in cooling slow impurity atoms has been discussed by Timmermans and Côté [9]. The main emphasis of our calculations is on the evaluation of the density profile of the fermionic component with varying temperature and composition for values of the coupling strengths relevant to a mixture of ^{39}K and ^{40}K atoms. We also identify two parameters which govern the behaviour of the profile. In the limit of the Thomas-Fermi approximation at zero temperature we recover the equations used by Mølmer [10] to describe the ground state of mixtures of bosons and fermions. Studies of the thermodynamic properties of ideal Fermi gases in harmonic traps have been reported by Butts and Rokhsar [11] and by Schneider and Wallis [12].

Interaction effects are very small in the normal phase but become significant as condensation induces a density increase of the bosonic component near the centre of the trap. For values of the (repulsive) coupling strengths in the range of present interest, the condensate pushes both the bosonic noncondensate and the fermionic fluid towards the periphery of the trap. With regard to the latter fluid, such 'squeezing' drives an increase in its chemical potential. As we shall see below, these effects on the fermionic density profile are especially striking in boson-rich mixtures, but rather low temperatures relative to the BEC transition need to be reached. Of course, an increase of the fermion-boson coupling, as may be achieved by modifying the scattering lengths with external fields [13, 14] and by changing the parameters of the trap or the components of the mixture, will enhance the BEC-induced changes in the fermionic fluid.

In the following we shall assume that the number of bosons in the trap is large enough that the kinetic energy term in the Gross-Pitaevskii equation for the wave function $\Psi(\mathbf{r})$ of the condensate can be neglected (see e.g. [15]). This corresponds to the so-called Thomas-Fermi limit and is in general a good approximation except in the immediate neighbourhood of the BEC transition temperature. It yields the strong-coupling result

$$\Psi^2(r) = [\mu_b - V_b^{ext}(r) - 2gn_{nc}(r) - fn_f(r)]/g \tag{1}$$

when the quantity in the square bracket is positive, and $\Psi^2(r) = 0$ otherwise. Here, $g = 4\pi\hbar^2 a_b/m_b$ and $f = 2\pi\hbar^2 a_f/m_r$ with a_f and a_b the boson-boson and boson-fermion s-wave scattering lengths and $m_r = m_b m_f/(m_b + m_f)$ with m_b and m_f the atomic masses; $\mu_b(T)$ is the chemical potential of the bosons at temperature T, $V_b^{ext}(r) = m_b\omega_b^2 r^2/2$ is a spherically symmetric external potential confining the bosons, $n_{nc}(r)$ is the average distribution of non-condensed bosons and $n_f(r)$ is that of the fermions. The factor 2 in the third term on the RHS of eqn (1) arises from exchange [16] and we have neglected a term involving the off-diagonal density of non-condensed bosons.

As already proposed in early work on the confined Bose fluid [17 - 19], we treat both the non-condensed bosons and the fermions as ideal gases in effective potentials $V_b^{eff}(r)$ and $V_f^{eff}(r)$ involving the relevant interactions. We write

$$V_b^{eff}(r) = V_b^{ext}(r) + 2g\Psi^2(r) + 2gn_{nc}(r) + fn_f(r) \tag{2}$$

and

$$V_f^{eff}(r) = V_f^{ext}(r) + f\Psi^2(r) + fn_{nc}(r) \ , \tag{3}$$

with $V_f^{ext}(r) = m_f\omega_f^2 r^2/2$. We are taking the fermionic component as a dilute, spin-polarized Fermi gas: the fermion-fermion interactions are then associated at leading order with p-wave scattering and are demonstrably negligible at the temperatures of present interest [11, 20]. We may then evaluate the thermal averages with standard Bose-Einstein and Fermi-Dirac distributions, taking the non-condensed particles to be in thermal equilibrium with the condensate at the same chemical potential $\mu_b(T)$ and the fermions at chemical potential $\mu_f(T)$. In the semiclassical approximation we obtain

$$n_f(r) = \frac{1}{h^3}\int d^3p \left\{\exp\left[\left(\frac{p^2}{2m_f} + V_f^{eff}(r) - \mu_f\right)/k_BT\right] + 1\right\}^{-1} \tag{4}$$

and

$$\begin{aligned} n_{nc}(r) &= \frac{1}{h^3}\int d^3p \left\{\exp\left[\left(\frac{p^2}{2m_b} + V_b^{eff}(r) - \mu_b\right)/k_BT\right] - 1\right\}^{-1} \\ &= \left(\frac{2\pi m_b k_B T}{h^2}\right)^{3/2} \sum_{j\geq 1} \frac{\exp[-j(V_b^{eff}(r)-\mu_b)/k_BT]}{j^{3/2}} \ . \end{aligned} \tag{5}$$

The chemical potentials are determined from the total numbers of bosons and fermions,

$$N_b = \int d^3r\, [\Psi^2(r) + n_{nc}(r)] \tag{6}$$

and

$$N_f = \int d^3r\, n_f(r) \ . \tag{7}$$

These equations complete the self-consistent closure of the model.

Before presenting relevant illustrative examples of the full numerical solution of the set of equations (1) - (7), it is useful to discuss a simplified form of the present three-fluid model (see also [7]). This is obtained by introducing an approximation which preserves only the repulsions exerted by the condensate: namely, we set to zero the last two terms in the RHS of eqns (1) and (2) and the last term in the RHS of eqn (3). Evidently, this approximation rests on the fact that both the non-condensed and the fermion component are very dilute gases and becomes all the more accurate as one moves towards boson-rich mixtures well below the BEC transition temperature. In this approximation we can (i) introduce a temperature-dependent scale length $R = (2\mu_b/m_b\omega_b^2)^{1/2}$ defining the radius outside which the condensate density vanishes, and (ii) scale the effective potential acting on the fermions by writing it in the form $V_f^{eff}(r) = \hbar\omega_f \tilde{V}_f^{eff}(x)$ where $x = r/R$ and

$$\tilde{V}_f^{eff}(x) = \begin{cases} \frac{1}{2}\gamma\left[\lambda + (1-\lambda)x^2\right] & \text{for} \quad x < 1 \\ \frac{1}{2}\gamma x^2 & \text{for} \quad x > 1 \end{cases} \tag{8}$$

with

$$\lambda = \frac{f m_b \omega_b^2}{g m_f \omega_f^2} \tag{9}$$

and

$$\gamma = \frac{2\mu_b m_f \omega_f}{\hbar m_b \omega_b^2} = \left[15 N_c a_b \left(\frac{m_b \omega_b}{\hbar}\right)^{1/2}\right]^{2/5} \frac{m_f \omega_f}{m_b \omega_b} \, . \tag{10}$$

Evidently, the dimensionless constant λ controls the shape of the effective potential seen by the fermions and hence their density profile: it depends only on (i) the ratio of the two relevant scattering lengths and (ii) the ratio of the spring constants of the two traps. Instead the parameter γ, which depends on the number $N_c(T)$ of bosons in the condensate through their chemical potential, controls the depth of the effective potential (in units of $\hbar\omega_f$). It is easily seen from eqn (8) that for $\lambda > 1$ $\tilde{V}_f^{eff}(x)$ decreases from the value $\gamma\lambda/2$ at the centre of the trap towards its minimum value $\gamma/2$ at $r = R$, and increases thereafter because of the confinement. In this regime the fermions are squeezed away from the centre of the trap into a shell overlying both the outer part of the condensate and the non-condensate. On the other hand, for $\lambda < 1$ the minimum value of $\tilde{V}_f^{eff}(x)$ is $\gamma\lambda/2$ at the centre of the trap: namely, in this regime the condensate merely raises the bottom of the confining well for the fermions without changing the sign of its central curvature.

The calculations that we report below refer to the fermion density profiles in a trap with $\omega_f = \omega_b = 100\,\mathrm{s}^{-1}$. We shall first consider (left panels in Figures 1 and 2) the case $a_b \simeq 80$ and $a_f \simeq 46$ Bohr radii for the boson-boson and boson-fermion s-wave scattering lengths, corresponding to the ^{39}K-^{40}K mixture [21]. With the above values we find $f \simeq 0.57g$ and hence $\lambda < 1$. We have also examined the regime $\lambda > 1$ by assuming $f = 2g$ (right panels in the Figures). We have studied the dependence of the profiles on the composition of the mixture by considering two cases, namely (i) $N_f = 10^3$ and $N_b = 10^6$ (top panels in the Figures) and (ii) $N_f = N_b = 10^4$ (bottom panels). The two characteristic temperatures of the mixture shown in the Figures are the BEC transition temperature $k_B T_c = \hbar\omega_b (N_b/\zeta(3))^{1/3}$ for an harmonically confined ideal Bose gas and the Fermi temperature T_f. The latter has been calculated from the chemical potential of the fermions in the simplified model at zero temperature. The increase of T_f due to the boson-fermion interactions, relative to the confined ideal-gas value $k_B T_f = \hbar\omega_f (6N_f)^{1/3}$, is quite large at boson-rich compositions (about 40% in Figure 1.a and 86% in Figure 1.c).

Figure 1 compares our results for the density profile of the fermions at two temperatures below T_c with those for a confined Fermi gas in the absence of all interactions. In this range of parameters the results obtained in the simplified model leading to eqn (8) are practically indistinguishable from those obtained from the full numerical solution of eqns (1) - (7). The interactions induce major distortions of the fermion density profile near the centre of the trap in the ^{39}K-^{40}K mixture at low temperatures and at boson-rich compositions (see the curve in Figure 1.a referring to $T/T_c = 0.1$ and $N_f = 10^{-3} N_b$). The transition from the first to the second regime of coupling strength λ is clearly shown by the comparison between the left and right-hand panels in Figure 1. For boson-rich compositions at low temperature, the fermions are in fact almost wholly expelled from the central region of the trap (see Figure 1.c). This agrees with the results of the ground-state calculations of Mølmer [10]. The density profiles of the bosons, that we do not show, are instead hardly affected by the presence of the fermions in the range of parameters that we have explored.

It is also interesting to point out that for $T = 0.1T_c$ the conditions of Figures 1.a and 1.c correspond to temperatures of the same order as the Fermi temperature T_f. In this case the effects of the interactions are more important than those due to the quantum degeneracy of the Fermi gas. On the contrary, the conditions of Figures 1.b and 1.d at $T = 0.1T_c$ correspond to temperatures much smaller than T_f and the effects of quantum degeneracy are much more important, as is illustrated by the comparison with the density profile for an ideal Boltzmann gas at the same

temperature (dots in Figures 1.a and 1.b).

Figure 2 shows the behaviour of the density $n_f(r=0)$ of fermions at the centre of the trap as a function of temperature, for the same coupling strengths and compositions as in Figure 1. In Figure 2.a we have reported in an inset the behaviour of the temperature derivative of $n_f(r=0)$, to display its upturn occurring as quantum degeneracy develops at sufficiently low values of T/T_f. Major effects should be expected in boson-rich mixtures if the coupling strength can be driven into the $\lambda > 1$ regime, as is seen from Figure 2.c.

In summary, we have studied the equilibrium density profile of a fermionic fluid in a confined, Bose-condensed mixture of bosons and fermions in dependence of composition and temperature. The fermion density at the centre of the trap can be used to detect the onset of degeneracy in the Fermi gas with decreasing temperature. Although we have assumed spherically symmetric traps, the model can easily be extended to asymmetric confinements through a simple change of variables.

As a final remark we notice that the density profile that we have calculated for the fermionic component immediately yields a semiclassical density of states $\rho_f(E)$ for the calculation of thermodynamic properties through the relation

$$\rho_f(E) = 2\pi(2m_f/h^2)^{3/2} \int d^3r[E - V_f^{eff}(r)]^{1/2} \ . \tag{11}$$

A similar relation holds, of course, for the density of states of the non-condensate [17-19, 7]. In the simplified model leading to eqn (8), that we have seen to be quite accurate compared with a fully self-consistent treatment of the mixture in the range of parameters that we have explored, the integral in eqn (11) is easily evaluated analytically. Calculations of thermodynamic properties for boson-fermion mixtures will be reported elsewhere.

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Figure captions

- Figure 1. Fermion density profile $n_f(r)$ (in units of a_0^{-3}, with $a_0 = (\hbar/m_b\omega)^{1/2}$ and ω the characteristic frequency of the harmonic trap) *versus* distance r from the centre of the trap (in units of a_0), for two values of the reduced temperature T/T_c ($T/T_c = 0.1$ and 0.5). The dashed curves and the dots are for an ideal Fermi gas and for an ideal Boltzmann gas (at $T/T_c = 0.1$) in the absence of bosons, respectively. The full curves are the results of the numerical solution of the full set of eqns (1) - (7). The values of the parameters for the various panels are as follows: (a) $f = 0.57g$, $N_f = 10^3$ and $N_b = 10^6$; (b) $f = 0.57g$ and $N_f = N_b = 10^4$; (c) $f = 2g$, $N_f = 10^3$ and $N_b = 10^6$; (d) $f = 2g$ and $N_f = N_b = 10^4$. The values of the BEC transition temperature T_c and of the Fermi temperature T_f are also indicated.

- Figure 2. Fermion density $n_f(0)$ at the centre of the trap (in units of a_0^{-3}) *versus* reduced temperature $k_BT/\hbar\omega$. The results of the simplified model in eqn (8) (long-dashed curves) are compared with those for an ideal Fermi gas (short-dashed curves). The arrows mark the BEC transition temperature and the Fermi temperature of the mixture. The inset in panel (a) shows the temperature derivative of $n_f(0)$ (in reduced units) versus reduced temperature.